

NOTRUMP, An Updated Version
Of TRUMP

Lewis D. Thorson

September 29, 1980



Lawrence
Livermore
Laboratory

This is an informal report intended primarily for internal or limited external distribution. The opinions and conclusions stated are those of the author and may or may not be those of the Laboratory.

This work was supported by the United States Nuclear Regulatory Commission under a Memorandum of Understanding with the United States Department of Energy.

CIRCULATION COPY
SUBJECT TO RECALL
IN TWO WEEKS

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This report has been reproduced
directly from the best available copy.

Available to DOE and DOE contractors from the
Office of Scientific and Technical Information
P.O. Box 62, Oak Ridge, TN 37831
Prices available from (615) 576-8401, FTS 626-8401

Available to the public from the
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Rd.,
Springfield, VA 22161

TABLE OF CONTENTS

	Page
Abstract	1
Introduction	1
Changes to BLOCK 1	2
Changes to BLOCK 9	3
The New BLOCK 11	3
BLOCK 1. Problem Controls, Limits, and Constants (Required)	4
BLOCK 9. Initial Conditions and Heat Generation Rates	12
BLOCK 11. Controls for Nodes to be Output for Plotting	13
AFTER - A Code to Manipulate BLOCK 11 Files	15

ABSTRACT

We describe a new version of the TRUMP¹ computer code, NOTRUMP, which runs on both the CDC-7600 and CRAY-1. There are slight differences in the input and major changes in output capability. A postprocessor, AFTER, is available to manipulate some of the new output features. Old data decks for TRUMP will normally run with only minor changes.

INTRODUCTION

The impetus for a new version of TRUMP arose from a desire to make the code machine-independent, to update the graphics capability, and to selectively suppress the large amounts of output generated by large long running problems. Every effort has been made to assure that old input decks will remain compatible.

The virtue of making the code machine-independent are two-fold. First, all present and future machines will be usable by recompiling. Second, much larger and longer problems can be run on the CRAY-1. Potential problem size is about doubled. Speedups of 2 are common and for certain problems this can be as high as 4 to 5.

The graphics have been entirely removed from the main code. Instead two separate files can be written which contain time and temperature information and allow for graphical manipulation in a postprocessor.

A major departure from the original TRUMP philosophy is that all data must be in a single data deck. Therefore use of control cards such as *INPUT, and *MAST is no longer possible. It was felt that these activities are more appropriate to a preprocessor. Most of the coding necessary to do these things still exist, and could be reactivated if there were a pressing need.

Since not all the possible options have been tried, it is possible that problems may arise. This is most likely in terms of the various TRUMP control cards. Many of these are somewhat out of date and not applicable in the context of the new version, such as having a single data deck. If problems do arise due consideration will be taken to rectify the situation.

Changes to BLOCK 1

Several new fields have been added to BLOCK 1, but they are invisible to the user unless explicitly invoked. The primary aim is to reduce the amount of output that is normally associated with a run. This is especially useful when making a parameter study. Once it is clear that the problem is set up correctly the volume of output can be drastically cut.

The same holds true with regard to error messages caused by input to the various BLOCKs. Usually a large number of errors are related to a single mistake and a few are enough to isolate the problem.

Another change allows one to reset certain classes of special nodes back to regular for each continuation problem. In certain types of problems this affords a significant improvement in both run time and accuracy.

The last change allows one to use several BLOCK 1's to specify a new KSPEC for different parts of a problem. This can be a significant help in run time by avoiding the reclassification of nodes with large time constants.

Changes to BLOCK 9

BLOCK 9 is used either to preset the initial conditions for selected nodes or to restart a problem from a previous run. The code will output the BLOCK 9 information when NPUNCH in BLOCK 1 is set, or by using the teletype option "BLK9" during the run. The information is written to a file called "BLOCK9".

A new field has been added which outputs the temperature, TT, with much more significance than was previously available. When NOTRUMP reads the BLOCK 9 input this new field is used if nonzero regardless of the first TT field. This is especially useful in "hard" problems where small changes in temperature result in small time steps.

Note that if a BLOCK9 file is written it must be incorporated into one data deck that is the input to a new NOTRUMP run.

The New BLOCK 11

In the past graphics were contained in the main code. This is not satisfactory except for simple geometries and does not allow the flexibility that is often desirable. It also requires modifications to the main code each time a new option is needed.

Hence we have completely rewritten the BLOCK 11 subroutine to create two files containing "PLOT" nodes and "DUMP" nodes for postprocessor routines. The reason for taking this activity out of the main code is twofold. First, the plot information can be manipulated in many ways without rerunning a problem. Second, it is difficult to produce a generalized contour routine

that can handle the generalized geometry and node numbering schemes that the code can handle. It seemed simpler to place the responsibility for producing contour plots on the user.

The "PLOT" node file contains a set of node temperatures and time for every cycle. This is similar to NUM in BLOCK 1, but the information is contained in a separate file. The maximum number of nodes written to the plot file is 32, but this can be changed by setting ISPSIZE in subroutine PLOT to the size desired and recompiling. The files created are a sequential family starting with PLOT**0.

The "DUMP" node file contains most or all the node temperatures at selected cycles or times. From this information the postprocessor can produce contour plots. The files created are a sequential family starting with DUMP**0.

Each problem or continuation problem can produce plot and/or dump file(s) as needed. There is no carryover of BLOCK 11 in a continuation problem.

A separate code, AFTER, is available that will manipulate both the PLOT and DUMP files. A short description appears at the end of this report.

BLOCK 1. Problem Controls, Limits, and Constants (Required).

Card 1. Format (3I5,I1,I4,6I5). General Controls

IPRINT	Number of time steps between data output, in addition to output on first, second, and last time steps, and output controlled by TIMEP. IPRINT is not used if negative, zero, or unspecified.
--------	--

NUM Identification number of a node for which temperature, rate of temperature change, phase or reactant concentrations, heat-generation rate, and time will be written out after each time step. NUM will not be used if zero or unspecified.

KDATA Controls options on output data, normal amount (0), minimum (-1), or maximum (1). See Section II.C.17a of the TRUMP manual.

In addition it is possible to selectively control the output from BLOCKs 3, 4, 5 and 10, during the set-up phase and cycle 0 and last. This new form is KDATA = + ABCD.

The "-" gives the minimum output as before; in addition

A controls BLOCK 3 output

B controls BLOCK 4 output

C controls BLOCK 5 output

D controls BLOCK 10 output

The convention is to turn off the output according to the following table:

	<u>Turn off if A, B, C, D, is</u>			
set up	9	8		4
cycle 0	9	8	7	5
cycle last	9		7	6

The exceptions are:

- 1) BLOCK 3 is not taken out of the set-up.
- 2) BLOCK 4 always gives the minimum output on the last cycle
- 3) If A = 8 or 9 then no BLOCK 9 input is printed.

KSPECR used to reset to regular specified special nodes for a continuation problem.

=1 reset type 4 nodes (KSPEC=0) [NTYPE(N)=4]

=2 reset type 5 nodes (KSPEC=1) [NTYPE(N)=5]

=3 both 1 and 2

KSPEC Node classification and difference-equation control.

Normally zero or unspecified. If zero, regular nodes will be reclassified as special nodes only when necessary to maintain the stability limit above the time step, and the interpolation factor in the heat-balance difference equations may vary in the range 0.57 to 1.0. If negative, no nodes may be reclassified, and the steady-state criteria will not be used to end the problem. If positive nodes will be reclassified as special nodes as they are created. If 2, the interpolation factor will be fixed at 1.0, so that the backward difference method will be used. If 3, the interpolation factor will be fixed at 0.5, so that the central difference method will be used. Node classifications may be made individually in BLOCK 4 with KS. All nodes listed in BLOCK 6 are classified as special nodes. DELT0 and SMALL must be specified when KSPEC is positive.

MCYC Maximum allowed number of time steps. MCYC will not be used if zero or unspecified. If negative, problem will end after the first time step.

MSEC Maximum allowed machine time, in seconds. MSEC will not be used if zero or unspecified. If negative, problem will end after the first time step.

NPUNCH Causes a deck of punched cards in the format of BLOCK 9 to be produced when the problem is interrupted by Sense Switch 1 or ends normally, if nonzero. The data are the final values of T, A, B and G. The new BLOCK 9 may be inserted in the input deck, which may then be resubmitted to continue the problem.

NDOT Causes all time derivatives to be maintained at zero during the problem, if nonzero. Not normally used.

IRITE Not used in this version. See Block 11.

ITAPE Not used in this version. See Block 11.

TIMEP Problem time interval between data output, in addition to output on first, second, and last time steps, and output controlled by IPRINT and JPIC. TIMEP is ignored if negative, zero, or unspecified. Output will be written at exact multiples of TIMEP, if possible, by adjusting the time steps in the range from SMALL to DELT0. The adjustment is also limited to a range from $2/3$ to $3/2$ of the time step that would otherwise be used.

SCALE Scale factor. Set to 1.0 if negative, zero, or unspecified. Will be applied to all geometric input data in BLOCKs 4, 5 and 6 read in following this BLOCK 1 and preceding any other BLOCK 1 with a different scale factor. Lengths will be multiplied by SCALE, areas by $SCALE^2$, volumes by $SCALE^3$.

Card 2. Format (2I1,I3,I5, 7E10.3). Symmetry, Units, and Limits

KSPECN Controls the number of messages output when nodes are reclassified from regular to special. Output is limited to 2^{KSPECN} messages. If KSPECN = 0 then all messages are output.

NERRM Like KSPECN except this controls the number of error messages sent during set up. Output is limited to 2^{NERRM} messages for each BLOCK. If NERRM = 0 then all messages are output.

KD Symmetry type indicator: 1 for nonsymmetric, 2 for axisymmetric, 3 for centrisymmetric. Input values of DRAD in BLOCKs 4, 5, and 6 read in after BLOCK 1 will be replaced with DRAD, 2 DRAD, and 4 $DRAD^2$, respectively. KD is set to 1 if unspecified or zero (see Section II.C.4 of the TRUMP manual.)

KT Temperature scale indicator: 1 for Centigrade, 2 for Kelvin, 3 for Fahrenheit, 4 for Rankin. KT is set to 1 if unspecified or zero. (See Section II.C.2. of the TRUMP manual).

- DELTO Maximum allowed time step. May be used with SMALL to limit range of time step. Not usually needed. DELTO is set to 10^{12} if unspecified or not in the range from 10^{-10} to 10^{12} . DELTO must be specified if KSPEC is positive.
- SMALL Minimum allowed time step. May be used with DELTO to limit range of time step. Not usually needed. SMALL is set to 10^{-12} if less than 10^{-12} . If SMALL is unspecified, the program sets SMALL to 2/3 of 1% of the smallest time constant of any regular node in the system, if at least 1/4 of the nodes are regular nodes. SMALL should be specified in continuation problems of type 3 or 4, if not specified in the original BLOCK 1.
- TVARY Desired maximum temperature change in each time step. TVARY is set to 5.0 if unspecified or zero. Controls size of the time step between limits of SMALL and DELTO. Steady state cannot end the problem until the maximum temperature change is less than 0.001 TVARY for two successive time steps. The convergence criteria for the iterative calculation for special nodes are a change in the weighted average temperature change of all connected special nodes of less than $5(10^{-5}) \cdot \text{TVARY}$, and in the temperature change of any finite-volume special node of less than $5(10^{-4}) \cdot \text{TVARY}$.

TAU Initial problem time. Will be set to zero if unspecified.

TIMAX Maximum allowable problem time. TIMAX will not be used if zero or unspecified. If it is negative, problem will end after first time step.

TMIN Minimum allowable problem temperature. Will be set to -10^{12} if equal to or larger than TMAX. HMELT(N) in BLOCK 2 will be set to zero for any material for which TMELT(N) is less than TMIN.

TMAX Maximum allowable problem temperature set to 10^{12} if equal to or less than TMIN. HMELT(N) in BLOCK 2 will be set to zero for any material for which TMELT(N) is greater than TMAX.

Card 3. Format (8E10.2). System Constants

CARD 3 remains as described in the TRUMP writeup.

BLOCK 9. Initial Conditions and Constant Heat Generation Rates

Card 1. Format (3I5, 5X, 4E10.3, 4X, E16.8).

NOTE	Node identification number.
NSEQ	Number of additional nodes with identical initial conditions.
NADD	Increment between successive node numbers in sequence of NSEQ + 1 nodes generated when NSEQ is used.
TT	Initial temperature. TT is set to TONE (BLOCK 1) if not specified.
AA	Initial weight fraction of first chemical reactant. AA is set to ALONE (BLOCK 1) if not specified. AA may be used to specify the initial concentration of low-temperature phase in nodes of materials with specified values of TMELT and HMELT, if columns 67 through 71 of the Problem Name Card are "A=BL9". Otherwise, the concentration will be 1.0 for initial temperature at or below TMELT and 0.0 for initial temperature above TMELT. If a negative value of AA, or of BB below, is specified, and the node contains the corresponding reactant, the concentration will be set to zero during the first time step, and the heat of reaction will be converted to sensible heat. No further reaction will then take place. The resulting temperature change will be accurate only if the change in specific heat of the material is small over the temperature interval involved. The temperature will increase if the heat of reaction is negative, and decrease if the heat of reaction is positive.

- BB Initial weight fraction of second chemical reactant. BB is set to BONE (BLOCK 1) if not specified. BB may be negative (see AA above).
- GG Heat-generation rate. GG is set to GONE (BLOCK 1) if not specified. Has no effect if GT vs TVARG is specified for this node in BLOCK 8. Typical units: cal/sec-cm^3 .
- TT As above but with more significance. This field is filled in if one sets NPUNCH in BLOCK 1. This is useful when specifying an initial temperature field for a new problem, especially if large gradients exist.

BLOCK 11. Controls for Nodes to be Output for Plotting

Card 1. Format (8I5, 4E10.3) Controls

- M11S Number of plot nodes, to a maximum of 32. These are the nodes output every time step. The maximum number can be reset by changing ISPSIZE in subroutine PLOT and recompiling.
- M11D Number of dump nodes; maximum is all the nodes in a problem.
- IALL = 1 to output all the nodes in a problem as dump nodes. In this case it is not necessary to specify M11D or to provide a list of the desired nodes.
- NUMPLOT Number of times to output the dump nodes. Necessary so a file of the proper size can be created.
- NUMPLOTS Number of times to output the plot nodes. Necessary so a file of the proper size can be created.
- JPIC Number of cycles between output of dump nodes. This can be changed during a run by using one of the teletype options.

ISHORT Used to inhibit short edits (KDATA negative in BLOCK 1) if
 dump nodes are to output as a function of time. Short edits
 will be output only every ISHORT times. Default = 1. This
 can also be used to suppress temperature information on short
 edits but still get boundary node data at frequent intervals.

ITIME =1 to force the Dump nodes to be output with time edits. If
 specified JPIC = 10000.

FTIME1 Conversion factors applied to time for both plot and dump
FTIME2 node output.
 $\text{time} = \text{FTIME1} + \text{FTIME2} * \text{time}$
 Default FTIME2 = 1.

FTEMP1 Conversion factors applied to temperature for both plot and
FTEMP2 dump node output
 $\text{temperature} = \text{FTEMP1} + \text{FTEMP2} * \text{TEMP}$
 Default FTEMP2 = 1.

Card 2, 3. Format (16I5) Plot Node List

This is a list of the nodes to be included in the Plot node file. There must be two cards since the code looks for 32 values. Only the first M11S values are used. If M11S=0 no data cards are needed.

Card 4. Format (16I5) Dump Node List

This is a list of the nodes to be included in the Dump node file. Only as many cards as required to input M11D nodes. If IALL = 1, no cards are necessary.

FORMAT FOR BLOCK 11 FILES

The BLOCK 11 files are FORTLIB Absolute files. There is a code, AFTER, which will manipulate them, but the file structure is included here for completeness.

a) PLOT**0, the "PLOT" node file

Word 1 - number of cycles the problem ran (NUMSP)

2 - M11S

3 - maximum number of nodes output each cycle

4 - 25 - problem name

26-57 - the node numbers

58 - end -have NUMSP groups of 33 words in each group word 1 is the time and the next 32 are the temperatures for each cycle.

b) DUMP**0, the "DUMP" node file

Word 1 - number of dumps (NUMD)

2 - M11D

3 - M11D

4-25 - Problem name

26 - M11D+26 - the node numbers

M11D+26 - end - Have NUMD groups of M11D+1 words. In each group word 1 is the time and the next M11D are the temperatures for each dump.

AFTER - A Code to Manipulate BLOCK 11 Files

AFTER was written to exploit the information in the BLOCK 11 files. A source is available from the author. It is not intended to be a static code, but rather one that will be tailored to meet specific needs and desires. It has certain basic capabilities which are useful in most situations.

Plot nodes can be handled in one of two ways. First a listing of some or all the node temperatures versus time can be produced. This information can then be fed into many available plot codes. Second temperature versus time plots can be produced for all the nodes. These are crude plots but can give a quick look at how a problem ran and also serve to delineate ranges of time that are of interest.

Dump nodes can either be listed or contoured. To contour requires the user to provide a subroutine, DECODE, to define how the node numbers are to be used in contouring. The code can also be used to generate a list of nodes and times and input these into the plotting code of choice.

In most cases the code can be used with little or no modification. However, this depends on the specific use intended.

Reference:

1. A. L. Edwards, "TRUMP: A Computer Program for Transient and Steady-State Temperature Distributions in Multidimensional Systems," UCRL 14754, Rev. III, September 1972, Lawrence Livermore Laboratory.